

D-proline, n-methoxycarbonyl-, undecyl ester

Inchi: InChI=1S/C18H33NO4/c1-3-4-5-6-7-8-9-10-11-15-23-17(20)16-13-12-14-19(16)18(21)22
InchiKey: NWOIUIKGJANZTI-UHFFFAOYSA-N
Formula: C18H33NO4
SMILES: CCCCCCCCCCOC(=O)C1CCCN1C(=O)OC
Mol. weight [g/mol]: 327.46

Physical Properties

Property code	Value	Unit	Source
logp	4.291		Crippen Method
mcvol	278.480	ml/mol	McGowan Method
rinpol	2222.00		NIST Webbook
rinpol	2222.00		NIST Webbook
tf	315.57	K	Cheméo Relay (1.0)

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320794&Units=SI>
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point

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<https://www.chemeo.com/cid/62-141-6/D-proline-n-methoxycarbonyl-undecyl-ester.pdf>

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